

Inorganic Components in Coal and Their Behavior at Elevated Temperatures

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The unexpected behavior of inorganic components in coal at elevated temperatures has humbled many researchers and technology developers. Many coal utilization technologies are developed with out an adequate assessment of the impacts of the inorganic components present in coal. The abundance and forms of inorganic components vary between coal types, coal seams and within the seams. Subbituminous and lignitic type coals contain organically associated and minerals. Bituminous and anthracite coals contain mainly minerals. During heating the inorganic components are transformed to gases, liquids, and solids. The characteristics of the inorganic gases, liquids, and solids reflect the association and abundance of the inorganic components in the coal and system conditions such as temperature and gas composition. Analysis of fly ash produced during combustion is highly complex and variable both in size and composition. Fly ash typically has a bimodal size distribution. The submicron size particles form as a result of condensation of flame-volatilized species upon gas cooling. The larger sized particles are derived from the non-volatile inorganic components. The physical and chemical properties of the ash intermediate species can cause significant challenges to the efficient and reliable operation of coal utilization technologies. The challenges include wear of system components, maintaining slag flow in wet bottom system, formation of deposits on heat transfer surfaces, formation of agglomerates in fluidized bed system, blinding and plugging of selective catalytic reduction systems for NO_x, and controlling the emission of toxic inorganic components. Many of the adverse impacts of inorganic components are being minimized through the use of more sophisticated methods of coal analysis and prediction. In addition, control technologies are being demonstrated to control the emission of volatile inorganic components such as mercury.

A full manuscript will be published in Fuel.

**Self assembly during the pyrolysis of coking coals and its
exploitation for the synthesis of new carbon materials
and nanomaterials**

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The formation of ordered carbon during the thermal treatment of some bituminous coals occurs by a unique natural process of discotic fluid self assembly and covalent capture. The report by Brooks and Taylor in 1965 of this ordered fluid intermediate, carbonaceous mesophase, represents the original discovery of the discotic nematic liquid crystalline phase. This talk will describe the origin, properties and behavior of carbonaceous mesophase and its relation to other discotic materials. The discotic assembly process occurring naturally in coal can also be systematically directed by templates and nanoconfined spaces to make unique supramolecular disk assemblies that can be converted to carbons by thermal treatment. The talk will discuss the synthesis of new carbon nanofibers and nanotubes as well as ordered and patterned thin films, whose graphene layer arrangements and properties can be molecularly engineered by this principle.

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Pyrolysis mechanisms of coal model compounds

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In the thermochemical conversion of coal, product formation is controlled by the relative rates of bond breaking, hydrogen donation, cross-linking, rearrangements, and mass transport. As a consequence of the structural complexity and heterogeneity of coal, it has been difficult to determine the reaction pathways at the molecular level. Thus, the pyrolysis of compounds that model key structural features found in coal has been studied to gain insight into the reaction pathways in coal, provide fundamental data for the development of kinetic models to describe the processing of coal at the molecular level, and provide fundamental knowledge to guide the design of more efficient strategies for the conversion of coal to higher value products. Over the past decade, our research group has focused on the impact of restricted mass transport on free radical reactions, reaction pathways of oxygen functional groups in low rank coal and lignin, and the role of carboxylic acids in cross-linking reactions in low-rank coal. Highlights from these mechanistic studies will be presented and its relevance to the thermal processing of coal discussed.

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Harold Schobert and the JP-900 Jet Fuel Program

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It is truly a pleasure to have been asked to contribute to this Storch Award symposium honoring Professor Harold Schobert. Some 12 years ago, I was approached by Harold who asked me if I was interested in joining a multi-disciplined research group that he was forming. He explained that the research group was going to attempt to make a new generation of thermally stable coal-based jet fuels that could withstand temperatures of 900°F (JP-900) and that my expertise as a polymer physical chemist could be useful in understanding the carbonaceous reactions that occur upon thermal degradation. My immediate reaction was, “he’s crazy”! 900°F, that’s almost 500°C! Surely there is no organic fuel that can withstand such temperatures. However, I agreed to join the group (I was a little short of research funds at the time!), and in this seminar I will describe how, with a little luck and perseverance, a JP-900 fuel was successfully developed.

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Extreme coalification: From lignite to anthracite in one career

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A retrospective and idiosyncratic review of coal chemistry. The specific emphasis focuses on (1) internal hydrogen transfer during coal reactions (without an external hydrogen source or hydrogen donors); (2) the role of net hydrogen as a correlative parameter for coal reactions; and (3) the advantages for coal conversion process development for producing high-value carbon products along with coal chemicals or liquid fuels. Examples will be drawn from the liquefaction chemistry of low-rank coals; co-coking of high-volatile bituminous coals for simultaneous production of coal-based jet fuel and needle coke; using medium-volatile bituminous coals as a source of hydrogen; and explorations of the chemistry of anthracite, including graphitization reactions.

A full manuscript will be published in *Fuel*.